MM 20: Computational Materials Modelling - Defect structure and formation

Time: Monday 17:00–18:15 Location: IFW B

MM 20.1 Mon 17:00 IFW B

Prediction of Morphologies at Inorganic/Organic Interfaces with Machine Learning on the Example of TCNE/Cu(111) — •Michael Scherbela, Lukas Hörmann, Veronika Obersteiner, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Many properties of thin films, such as their solubility or conductivity, depend strongly on the crystal structure of the adsorbed molecules. A major step towards designing new materials is therefore understanding and predicting the polymorphs that form at interfaces. This could in principle be done by finding low energy structures using ab-initio methods. However, the many degrees of freedom lead to a rich polymorphism that prohibits an exhaustive search for the global minimum. We show on the example of Tetracyanoethylene/Cu(111) that this challenge can be tackled with a combination of coarse-graining and machine learning:

First we determine adsorption geometries that isolated molecules adopt on the substrate. We then build supercells by combining these isolated adsorption geometries to generate a set of possible "guess polymorphs". This discretizes the configurational space to a huge, but finite size. Using optimal design methods we select a small, representative subset, calculate its energies using DFT and extract effective interactions between adsorbates. This provides an efficient energy prediction for all remaining guess polymorphs which is exploited by sampling the energetically most promising structures and iterated relearning. For TCNE/Cu(111), we predict stable polymorphs for different coverages and explain an experimentally observed phase transition.

MM 20.2 Mon 17:15 IFW B

Ab-initio study of the interplay of hydrogen and microstructure in Ni-based superalloys — •Poulumi Dey, Zahra Tarzimoghadam, Dirk Ponge, Eunan McEniry, Tilmann Hickel, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Ni-based superalloys with their excellent corrosion resistance are attractive for applications where exposure to hydrogen is inevitable such as sour gas environments in oilfields. The adverse impact of hydrogen on the desired mechanical properties of these alloys, however, often restricts the acceptable strength levels of these materials. In the present work, we perform ab-initio calculations to establish the fact that the delicate behavior of hydrogen sensitively depends on microstructure features present in the superalloy. In particular, we consider the volume fractions of different precipitate phases which can be experimentally adjusted by annealing and aging conditions. With the aid of density functional theory (DFT), we perform a quantitative analysis of the hydrogen solution enthalpies within the precipitates and their interface to the matrix material. The study thus provides crucial information about the impact of chemistry and crystal structure on the hydrogen solubility and diffusivity at the interfaces as well as possible nucleation points for hydrogen-induced fracture in the material.

MM 20.3 Mon 17:30 IFW B

Embedded-atom study of low-energy equilibrium triple junction structures and energies — •Sebastian Eich and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

We present an atomistic study of the structures and defect energies of iron triple junctions (TJs) in polycrystalline materials. Line energies of bulk TJs (merging three grain boundaries (GBs)) and surface TJs (merging one grain boundary and two surfaces) are found to be very low. In absolute value, they amount to only a few $10^{-10}\,\mathrm{Jm}^{-1}$. Remarkably, defined as a correct excess energy relative to the GBs, the bulk TJ energy is determined to be negative in all studied configurations with an average value of $-2.8\times10^{-10}\,\mathrm{Jm}^{-1}$. These quantitative results are in contrast to various experimental attempts, but they fully agree with simple geometric estimates.

Finally, we relate the negative TJ line energies to the excess segregation at TJs in a realistic Fe–Cr model system.

[1]: S. Eich, G. Schmitz, Embedded-atom study of low-energy equilibrium triple junction structures and energies, Acta Mater. 109 (2016) 364–374.

[2]: S. Eich, D. Beinke, G. Schmitz, Embedded-atom potential for an accurate thermodynamic description of the iron–chromium system, Comput. Mater. Sci. 104 (2015) 185–192.

MM 20.4 Mon 17:45 IFW B

Heterogeneous nucleation at prestructured seeds in Ni — •Grisell Diaz Leines, Ralf Drautz, and Jutta Rogal — Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

The fundamental principles of crystallization and polymorph selection in metals are largely determined during the early stages of nucleation. The presence of impurities and the crystallization conditions influence directly the microstructural evolution of the material. In this work we investigate the influence of small prestructured seeds on the nucleation mechanism during solidification in nickel. We employ transition path sampling simulations to enable the investigation of nucleation on the atomistic level. The analysis of the transition path ensemble obtained from our simulations indicates that, in comparison to homogeneous nucleation the presence of fcc and hcp seeds enhances the nucleation rate and determines the structure of the growing nuclei. Icosahedral and bcc seeds on the other hand have no effect on either the mechanism or the nucleation rates. Furthermore, we demonstrate that different conditions of undercooling and pressure determine the amount of hcp and fcc coordinated atoms that compose the growing nuclei and therefore the selected polymorph. Our results provide atomistic insight into the process of seeded heterogeneous nucleation at different crystallization conditions and shed light on the principles of polymorph selection in Ni.

MM 20.5 Mon 18:00 IFW B

Electrons and phonons on equal footing: Band renormalization in Diamondoids — •Pablo Risueno, Peng Han, and Gabriel Bester — UHH, Grindelallee 117, Hamburg, Germany

Recent work on electron-phonon coupling has considered the renormalization of the electronic states due to the interaction with the vibronic degrees of freedom. The complementary effect that electrons have on phonons has been mostly ignored. In turn, these renormalized phonon energies have a renormalization effect on the electronic states, which calls for a self-consistent treatment of electrons and phonons, treating both on equal footing. We will show how this self-consistent effect can be incorporated into the calculations and quantify its importance. We show results for small carbon clusters known as diamondoids, which are relevant in technological applications and are computationally tractable by our numerical approach.